

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.87	0.81	0.87	0.82	0.86	0.86

Model Results

Predicted value: 7.13e-03 mol/L

Global applicability domain: Inside

Local applicability domain index: 7.70e-01

Confidence level: 5.12e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>Oxydisulfoton</div> <div>Measured: 1.38e-02</div> <div>Predicted: 7.13e-03</div>	<div>Image not found</div> <div>Phorate sulfoxide</div> <div>Measured: 2.89e-02</div> <div>Predicted: 1.04e-02</div>	<div>Image not found</div> <div>Terbufos sulfoxide</div> <div>Measured: 3.61e-03</div> <div>Predicted: 3.26e-03</div>
<div>Image not found</div> <div>Thiodicarb</div> <div>Measured: 7.29e-05</div> <div>Predicted: 1.63e-04</div>	<div>Image not found</div> <div>Isothioate</div> <div>Measured: 3.73e-04</div> <div>Predicted: 2.34e-04</div>	